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Unleash the power of the amygdala: How to incorporate MedChem know-how early on in the CADD lead optimization phase

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Abstract

Given the amount of pressure under which pharmacompanies have to discover and develop potential drug candidates today, one ought to think about how to bring impetus into drug discovery pipelines these days: a) shorten the lead optimization cycle. It is more important than ever to quickly advance drug candidates to the clinical phases. b) Venture into unexplored chemical space. Chemical space occupied by existing drugs is increasingly tight, so the urge to get into new chemical classes with unexplored space is of paramount importance.

Thus, software enabling the Computational and Medicinal Chemist alike to put their knowledge into the compound design *at the same time* would render successive project meetings unnecessary. Both researchers would decide right in front of the computer which compounds to make next. The decision can be supported by prioritization, i.e. an estimate of how well the new compound(s) would bind with respect to the reference structure, provided a protein is present. This would provide more confidence in the decision and potentially less time spent synthesizing the wrong molecules.

LeadIT is scaffold hopping software that addresses the above mentioned criteria by incorporating years of research with researchers. Its interactive design unleashes MedChem know-how early on in the computational design phase and lets the team come up with tens of variations of the parent compounds in the matter of an afternoon.

The talk will highlight the conceptual design of the software with technical aspects as well as a few application scenarios to show-case its capabilities.

Biography

Carsten Detering has completed his PhD in Physical Chemistry from Freie Universitaet Berlin, Germany and postdoctoral studies from the University of Washington in Seattle, where he worked on the computational design of a new class of inhibitors for treatment of Malaria. He is the CEO of BioSolveIT Inc., the US daughter company of the Germany based BioSolveIT GmbH, the leader in fragment-based, synthesis backed ligand design.